Rafael Viruela

List of Publications by Year in Descending Order

69 papers	1,847 citations	25 h-index	40 g-index
70 ext. papers	1,911 ext. citations	5.7 avg, IF	3.79 L-index

#	Paper	IF	Citations
69	The Role of Planarity versus Nonplanarity in the Electronic Communication of TCAQ-Based Push-Pull Chromophores. *ChemPlusChem*, **2018**, 83, 300-307	2.8	12
68	Theoretical insights into the structural, electronic and optical properties of benzotrithiophene-based hole-transporting materials. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	3
67	Relationship between Electron Affinity and Half-Wave Reduction Potential: A Theoretical Study on Cyclic Electron-Acceptor Compounds. *ChemPhysChem*, **2016**, 17, 3881-3890	3.2	11
66	Efficient light harvesters based on the 10-(1,3-dithiol-2-ylidene)anthracene core. *Organic Letters*, **2013**, 15, 4166-9	6.2	16
65	A bis(triazole)benzamide receptor for the complexation of halide anions and neutral carboxylic acid guests. Guest-controlled topicity and self-assembly. *Organic and Biomolecular Chemistry*, **2013**, 11, 765-72	3.9	13
64	Donor-acceptors containing the 10-(1,3-dithiol-2-ylidene)anthracene unit for dye-sensitized solar cells. *Chemistry - A European Journal*, **2012**, 18, 11621-9	4.8	38
63	Bowl-shape electron donors with absorptions in the visible range of the solar spectrum and their supramolecular assemblies with C60. *Chemical Science*, **2012**, 3, 498-508	9.4	41
62	A fully conjugated TTF-TCAQ system: synthesis, structure, and electronic properties. *Chemistry - A European Journal*, **2011**, 17, 2957-64	4.8	24
61	A bis-exTTF macrocyclic receptor that associates C60 with micromolar affinity. *Journal of the American Chemical Society*, **2010**, 132, 1772-3	16.4	86
60	Diskrete supramolekulare Donor-Akzeptor-Komplexe. *Angewandte Chemie*, **2009**, 121, 829-834	3.6	17
59	Discrete supramolecular donor-acceptor complexes. *Angewandte Chemie - International Edition*, **2009**, 48, 815-9	16.4	102
58	Controlled self-assembly of electron donor nanotubes. *Organic Letters*, **2009**, 11, 4524-7	6.2	24
57	Weighting non-covalent forces in the molecular recognition of C(60). Relevance of concave-convex complementarity. *Chemical Communications*, **2008**, 4567-9	5.8	68
56	Aminopyrimidine-Based Donor-Acceptor Chromophores: Push-Pull versus Aromatic Behaviour. *European Journal of Organic Chemistry*, **2008**, 2008, 99-108	3.2	20
55	Concave tetrathiafulvalene-type donors as supramolecular partners for fullerenes. *Angewandte Chemie - International Edition*, **2007**, 46, 1847-51	16.4	113
54	Concave Tetrathiafulvalene-Type Donors as Supramolecular Partners for Fullerenes. *Angewandte Chemie*, **2007**, 119, 1879-1883	3.6	23
53	Synthesis and radical coupling of pyridine-bridged pi-extended tetrathiafulvalene (TTF)-type donors and push-pull analogues. *Organic and Biomolecular Chemistry*, **2007**, 5, 1201-9	3.9	14

52	Electronic interactions in a new pi-extended tetrathiafulvalene dimer. *Chemistry - A European Journal*, **2006**, 12, 2709-21	4.8	29
51	The interplay of inverted redox potentials and aromaticity in the oxidized states of new pi-electron donors: 9-(1,3-dithiol-2-ylidene)fluorene and 9-(1,3-dithiol-2-ylidene)thioxanthene derivatives. *Chemistry - A European Journal*, **2006**, 12, 3389-400	4.8	32
50	A study by spectroelectrochemical FTIR and density functional theory calculations of the reversible complexing ability of an electroactive tetrathiafulvalene crown. *Journal of Physical Chemistry A*, **2005**, 109, 1188-95	2.8	3
49	Raman and theoretical study of the solvent effects on the sizable intramolecular charge transfer in the push-pull 5-(dimethylamino)-5Snitro-2,2Sbithiophene. *Journal of Physical Chemistry A*, **2005**, 109, 8724-31	2.8	26
48	Highly conjugated p-quinonoid pi-extended tetrathiafulvalene derivatives: a class of highly distorted electron donors. *Chemistry - A European Journal*, **2004**, 10, 2067-77	4.8	27
47	A theoretical study of neutral and reduced tetracyano-p-quinodimethane (TCNQ). *Computational and Theoretical Chemistry*, **2004**, 709, 97-102		23
46	On the electron affinity of TCNQ. *Chemical Physics Letters*, **2004**, 391, 148-151	2.5	48
45	A new series of □extended tetrathiafulvalene derivatives incorporating fused furanodithiino and thienodithiino units: a joint experimental and theoretical study. *Journal of Materials Chemistry*, **2004**, 14, 2822-2830		16
44	Theoretical study of the molecular structure and the stability of neutral and reduced tetracyanoethylene. *Chemical Physics Letters*, **2003**, 375, 376-382	2.5	15
43	Theoretical description of the Raman spectrum of a vinylene-bridged quaterthiophene oligomer. *Journal of Molecular Structure*, **2003**, 651-653, 657-664	3.4	9
42	First signals of electrochemically oxidized species of TTF and TTM-TTF: A study by in situ spectroelectrochemical FTIR and DFT calculations. *Physical Chemistry Chemical Physics*, **2003**, 5, 4672-4679	3.6	24
41	Electronic spectra of tetrathiafulvalene and its radical cation: analysis of the performance of the time-dependent DFT approach. *Chemical Physics Letters*, **2002**, 352, 491-498	2.5	43
40	. *Chemistry - A European Journal*, **2000**, 6, 1199-1213	4.8	16
39	Theoretical and structural studies of lithium cyclic amide conformations. Monomers and aggregates. *Perkin Transactions II RSC*, **2000**, 1619-1624		5
38	Experimental and theoretical studies into thestructural perturbations between neutral, oxidised and reduced forms of 1,4-dithiinoquinoxalinederivatives. *Journal of Materials Chemistry*, **2000**, 10, 2448-2457		9
37	pi conjugation across the tetrathiafulvalene core: synthesis of extended tetrathiafulvalene derivatives and theoretical analysis of their unusual electrochemical properties. *Chemistry - A European Journal*, **2000**, 6, 1199-213	4.8	35
36	A New Type of □Electron Donors with One Dithiole Unit: Substituted 7-(1,3-Dithiol-2-ylidene)-7-hydrobenz[d,e]anthracenes. *European Journal of Organic Chemistry*, **1999** , 1999, 1239-1247	3.2	16
35	Flexibility of TTF. a theoretical study. *Synthetic Metals*, **1999**, 103, 1991-1992	3.6	34

34	Acene-type donors bearing one 1,3-dithiole ring. *Synthetic Metals*, **1999**, 102, 1635-1636	3.6	1
33	Effects of Carbon-sp3 Bridging on the Electronic Properties of Oligothiophenes. *Synthetic Metals*, **1999**, 101, 602-603	3.6	7
32	Benzoannulated quinone-type electron acceptors: evolution of the molecular and electronic structures upon reduction. *Computational and Theoretical Chemistry*, **1998**, 426, 135-143		
31	Donor–Acceptor Species Derived from Functionalised 1,3-Dithiol-2-ylidene Anthracene Donor Units Exhibiting Photoinduced Electron Transfer Properties: Spectroscopic, Electrochemical, X-Ray Crystallographic and Theoretical Studies. *Chemistry - A European Journal*, **1998**, 4, 2580-2592	4.8	50
30	Difficulties of density functional theory in predicting the torsional potential of 2,2?-bithiophene **1998**, 70, 303-312		31
29	New 1,3-dithiol-2-ylidene donor–acceptor chromophores with intramolecular charge-transfer properties, and related donor–donor molecules: synthesis, electrochemistry, X-ray crystal structures, non-linear optical properties and theoretical calculations. *Journal of Materials Chemistry*, **1998**, 8, 1173-1184		49
28	Synthesis, Properties, and Theoretical Characterization of Largely π-Extended Tetrathiafulvalene Derivatives with Quinonoid Structures. *Journal of Organic Chemistry*, **1998**, 63, 1268-1279	4.2	112
27	Reaction of C60with Sultines: Synthesis, Electrochemistry, and Theoretical Calculations of Organofullerene Acceptors. *Journal of Organic Chemistry*, **1997**, 62, 7585-7591	4.2	50
26	Geometric Structure and Torsional Potential of Biisothianaphthene. A Comparative DFT and ab Initio Study. *Journal of the American Chemical Society*, **1997**, 119, 1360-1369	16.4	89
25	Synthesis and Electrochemistry of Electronegative Spiroannelated Methanofullerenes: Theoretical Underpinning of the Electronic Effect of Addends and a Reductive Cyclopropane Ring-Opening Reaction. *Journal of the American Chemical Society*, **1997**, 119, 9871-9882	16.4	79
24	Synthesis, properties and charge transfer complexes of covalently attached [60]fullerene-tetrathiafulvalenes. *Journal of Physics and Chemistry of Solids*, **1997**, 58, 1713-1718	3.9	12
23	Synthesis, Characterization, and Theoretical Study of Sulfur-Containing Donor-Acceptor DCNQI Derivatives with Photoinduced Intramolecular Electron Transfer. *Journal of Organic Chemistry*, **1996**, 61, 3041-3054	4.2	16
22	Influence of Benzoannulation on the Molecular and Electronic Structures of Tetracyanoquinodimethanes. *The Journal of Physical Chemistry*, **1996**, 100, 6138-6146		34
21	Synthesis and Characterization of Novel Donor-Acceptor Naphthoquinone Derivatives with Photoinduced Charge-Transfer Properties. A Joint Experimental and Theoretical Study. *Journal of Organic Chemistry*, **1995**, 60, 5643-5650	4.2	25
20	Synthesis and Characterization of 11,11,12,12-Tetracyano-1,4-anthraquinodimethanes (1,4-TCAQs): Novel Electron Acceptors with Photoinduced Charge-Transfer Properties. *Journal of Organic Chemistry*, **1995**, 60, 4077-4084	4.2	17
19	Molecular and electronic structure of a largely extended tetracyanoquinodimethane. *Synthetic Metals*, **1995**, 70, 1031-1032	3.6	7
18	Electronic structure of novel phthalocyanine analogues containing the 1,2,4-triazole unit. *Synthetic Metals*, **1995**, 71, 2291-2292	3.6	17
17	6,11-Bis(dicyanomethylene)-12-methylbenzo[b]phenoxazine and 6,11-dicyanimino-12-methylbenzo[b]phenoxazine as novel donor–acceptor systems. *Journal of Materials Chemistry*, **1995**, 5, 1563-1570		6

16	New functionalized tetrathiafulvalenes: X-ray crystal structures and physico-chemical properties of TTFC(O)NMe2 and TTFC(O)OC4H9: a joint experimental and theoretical study. *Journal of Materials Chemistry*, **1995**, 5, 1689-1696		50
15	A theoretical study of the molecular and electronic structure of benzoannulated tetracyanoquinodimethanes. *Journal of Materials Chemistry*, **1995**, 5, 1697-1705		7
14	Influence of nitrogen substitution on the electronic band structure of poly(peri-naphthalene). *Synthetic Metals*, **1995**, 69, 705-706	3.6	1
13	The First sulfur-containing twin-DCNQI-type acceptor. *Advanced Materials*, **1994**, 6, 765-768	24	9
12	Single-Component Donor-Acceptor Organic Semiconductors Derived from TCNQ. *Journal of Organic Chemistry*, **1994**, 59, 4618-4629	4.2	42
11	Theoretical Studies of Chemical Interactions. Ab Initio Calculations on Lithium Dialkylamides and Their Carbonylation Reactions. *Journal of the American Chemical Society*, **1994**, 116, 10110-10116	16.4	14
10	Valence electronic structure of C60: Theoretical analysis of photoemission data. *Synthetic Metals*, **1993**, 56, 3246-3251	3.6	2
9	Geometric and electronic structure of dithiapyranylidine: evolution upon oxidation. *Synthetic Metals*, **1993**, 57, 4572-4578	3.6	
8	Valence bands of poly(methylmethacrylate) and photoion emission in vacuum ultraviolet region. *Journal of Applied Physics*, **1992**, 72, 5423-5428	2.5	20
7	Molecular orbital calculation of the soft-hard acidity of zeolites and its catalytic implications. *Journal of Catalysis*, **1992**, 136, 521-530	7.3	31
6	Theoretical EHT study of oxidative coupling of methane on pure MgO and MgO doped with Li and Na. *Journal of Molecular Catalysis*, **1991**, 64, 191-200		6
5	Theoretical eht study of isobutene adsorption on model clusters of first series transition metal oxides and MgO. *Journal of Molecular Catalysis*, **1988**, 43, 303-314		4
4	MINDO/3 Study of the Rearrangement of 1-Methylcyclohexyl Cation to 1,2-Dimethylcyclopentyl Cation. *Journal of Computational Chemistry*, **1986**, 7, 417-427	3.5	
3	Theoretical EHT study of propene adsorption on model clusters. *Journal of Molecular Catalysis*, **1986**, 34, 47-55		7
2	A proposal for a branching mechanism in medium-sized cycloalkanes: MINDO/3 study of the hypersurface for isomerization of cyclohexylium to 1-methylcyclopentylium ion. *Journal of the Chemical Society Perkin Transactions II*, **1986**, 49-53		8
1	Theoretical eht study of propene adsorption on model clusters of first series transition metal oxides and MgO. *Journal of Molecular Catalysis*, **1985**, 30, 81-93		8