

Rafael Viruela

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69
papers

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h-index

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70
ext. papers

1,911
ext. citations

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avg, IF

3.79
L-index

#	Paper	IF	Citations
69	Concave tetrathiafulvalene-type donors as supramolecular partners for fullerenes. <i>Angewandte Chemie - International Edition</i> , 2007 , 46, 1847-51	16.4	113
68	Synthesis, Properties, and Theoretical Characterization of Largely π -Extended Tetrathiafulvalene Derivatives with Quinonoid Structures. <i>Journal of Organic Chemistry</i> , 1998 , 63, 1268-1279	4.2	112
67	Discrete supramolecular donor-acceptor complexes. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 815-9	16.4	102
66	Geometric Structure and Torsional Potential of Bisothianaphthene. A Comparative DFT and ab Initio Study. <i>Journal of the American Chemical Society</i> , 1997 , 119, 1360-1369	16.4	89
65	A bis-exTTF macrocyclic receptor that associates C60 with micromolar affinity. <i>Journal of the American Chemical Society</i> , 2010 , 132, 1772-3	16.4	86
64	Synthesis and Electrochemistry of Electronegative Spiroannulated Methanofullerenes: Theoretical Underpinning of the Electronic Effect of Addends and a Reductive Cyclopropane Ring-Opening Reaction. <i>Journal of the American Chemical Society</i> , 1997 , 119, 9871-9882	16.4	79
63	Weighting non-covalent forces in the molecular recognition of C(60). Relevance of concave-convex complementarity. <i>Chemical Communications</i> , 2008 , 4567-9	5.8	68
62	Reaction of C60 with Sultines: Synthesis, Electrochemistry, and Theoretical Calculations of Organofullerene Acceptors. <i>Journal of Organic Chemistry</i> , 1997 , 62, 7585-7591	4.2	50
61	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. <i>Chemistry - A European Journal</i> , 1998 , 4, 2580-2592	4.8	50
60	New functionalized tetrathiafulvalenes: X-ray crystal structures and physico-chemical properties of TTF π (O)NMe ₂ and TTF π (O)O π 4H9: a joint experimental and theoretical study. <i>Journal of Materials Chemistry</i> , 1995 , 5, 1689-1696		50
59	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. <i>Journal of Materials Chemistry</i> , 1998 , 8, 1173-1184		49
58	On the electron affinity of TCNQ. <i>Chemical Physics Letters</i> , 2004 , 391, 148-151	2.5	48
57	Electronic spectra of tetrathiafulvalene and its radical cation: analysis of the performance of the time-dependent DFT approach. <i>Chemical Physics Letters</i> , 2002 , 352, 491-498	2.5	43
56	Single-Component Donor-Acceptor Organic Semiconductors Derived from TCNQ. <i>Journal of Organic Chemistry</i> , 1994 , 59, 4618-4629	4.2	42
55	Bowl-shape electron donors with absorptions in the visible range of the solar spectrum and their supramolecular assemblies with C60. <i>Chemical Science</i> , 2012 , 3, 498-508	9.4	41
54	Donor-Acceptors containing the 10-(1,3-dithiol-2-ylidene)anthracene unit for dye-sensitized solar cells. <i>Chemistry - A European Journal</i> , 2012 , 18, 11621-9	4.8	38
53	π conjugation across the tetrathiafulvalene core: synthesis of extended tetrathiafulvalene derivatives and theoretical analysis of their unusual electrochemical properties. <i>Chemistry - A European Journal</i> , 2000 , 6, 1199-213	4.8	35

52	Flexibility of TTF. a theoretical study. <i>Synthetic Metals</i> , 1999 , 103, 1991-1992	3.6	34
51	Influence of Benzoannulation on the Molecular and Electronic Structures of Tetracyanoquinodimethanes. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 6138-6146		34
50	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. <i>Chemistry - A European Journal</i> , 2006 , 12, 3389-400	4.8	32
49	Difficulties of density functional theory in predicting the torsional potential of 2,2'-bithiophene 1998 , 70, 303-312		31
48	Molecular orbital calculation of the soft-hard acidity of zeolites and its catalytic implications. <i>Journal of Catalysis</i> , 1992 , 136, 521-530	7.3	31
47	Electronic interactions in a new pi-extended tetrathiafulvalene dimer. <i>Chemistry - A European Journal</i> , 2006 , 12, 2709-21	4.8	29
46	Highly conjugated p-quinonoid pi-extended tetrathiafulvalene derivatives: a class of highly distorted electron donors. <i>Chemistry - A European Journal</i> , 2004 , 10, 2067-77	4.8	27
45	Raman and theoretical study of the solvent effects on the sizable intramolecular charge transfer in the push-pull 5-(dimethylamino)-5-nitro-2,2'-bithiophene. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 8724-31	2.8	26
44	Synthesis and Characterization of Novel Donor-Acceptor Naphthoquinone Derivatives with Photoinduced Charge-Transfer Properties. A Joint Experimental and Theoretical Study. <i>Journal of Organic Chemistry</i> , 1995 , 60, 5643-5650	4.2	25
43	A fully conjugated TTF-TCNQ system: synthesis, structure, and electronic properties. <i>Chemistry - A European Journal</i> , 2011 , 17, 2957-64	4.8	24
42	Controlled self-assembly of electron donor nanotubes. <i>Organic Letters</i> , 2009 , 11, 4524-7	6.2	24
41	First signals of electrochemically oxidized species of TTF and TTM-TTF: A study by in situ spectroelectrochemical FTIR and DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2003 , 5, 4672-4679	3.6	24
40	Concave Tetrathiafulvalene-Type Donors as Supramolecular Partners for Fullerenes. <i>Angewandte Chemie</i> , 2007 , 119, 1879-1883	3.6	23
39	A theoretical study of neutral and reduced tetracyano-p-quinodimethane (TCNQ). <i>Computational and Theoretical Chemistry</i> , 2004 , 709, 97-102		23
38	Aminopyrimidine-Based Donor-Acceptor Chromophores: Push-Pull versus Aromatic Behaviour. <i>European Journal of Organic Chemistry</i> , 2008 , 2008, 99-108	3.2	20
37	Valence bands of poly(methylmethacrylate) and photoion emission in vacuum ultraviolet region. <i>Journal of Applied Physics</i> , 1992 , 72, 5423-5428	2.5	20
36	Diskrete supramolekulare Donor-Akzeptor-Komplexe. <i>Angewandte Chemie</i> , 2009 , 121, 829-834	3.6	17
35	Synthesis and Characterization of 11,11,12,12-Tetracyano-1,4-anthraquinodimethanes (1,4-TCAQs): Novel Electron Acceptors with Photoinduced Charge-Transfer Properties. <i>Journal of Organic Chemistry</i> , 1995 , 60, 4077-4084	4.2	17

34	Electronic structure of novel phthalocyanine analogues containing the 1,2,4-triazole unit. <i>Synthetic Metals</i> , 1995 , 71, 2291-2292	3.6	17
33	Efficient light harvesters based on the 10-(1,3-dithiol-2-ylidene)anthracene core. <i>Organic Letters</i> , 2013 , 15, 4166-9	6.2	16
32	A new series of π -extended tetrathiafulvalene derivatives incorporating fused furanodithiino and thienodithiino units: a joint experimental and theoretical study. <i>Journal of Materials Chemistry</i> , 2004 , 14, 2822-2830		16
31	. <i>Chemistry - A European Journal</i> , 2000 , 6, 1199-1213	4.8	16
30	A New Type of π -Electron Donors with One Dithiole Unit: Substituted 7-(1,3-Dithiol-2-ylidene)-7-hydrobenz[d,e]anthracenes. <i>European Journal of Organic Chemistry</i> , 1999 , 1999, 1239-1247	3.2	16
29	Synthesis, Characterization, and Theoretical Study of Sulfur-Containing Donor-Acceptor DCNQI Derivatives with Photoinduced Intramolecular Electron Transfer. <i>Journal of Organic Chemistry</i> , 1996 , 61, 3041-3054	4.2	16
28	Theoretical study of the molecular structure and the stability of neutral and reduced tetracyanoethylene. <i>Chemical Physics Letters</i> , 2003 , 375, 376-382	2.5	15
27	Synthesis and radical coupling of pyridine-bridged π -extended tetrathiafulvalene (TTF)-type donors and push-pull analogues. <i>Organic and Biomolecular Chemistry</i> , 2007 , 5, 1201-9	3.9	14
26	Theoretical Studies of Chemical Interactions. Ab Initio Calculations on Lithium Dialkylamides and Their Carbonylation Reactions. <i>Journal of the American Chemical Society</i> , 1994 , 116, 10110-10116	16.4	14
25	A bis(triazole)benzamide receptor for the complexation of halide anions and neutral carboxylic acid guests. Guest-controlled topicity and self-assembly. <i>Organic and Biomolecular Chemistry</i> , 2013 , 11, 765-779	3.9	13
24	The Role of Planarity versus Nonplanarity in the Electronic Communication of TCAQ-Based Push-Pull Chromophores. <i>ChemPlusChem</i> , 2018 , 83, 300-307	2.8	12
23	Synthesis, properties and charge transfer complexes of covalently attached [60]fullerene-tetrathiafulvalenes. <i>Journal of Physics and Chemistry of Solids</i> , 1997 , 58, 1713-1718	3.9	12
22	Relationship between Electron Affinity and Half-Wave Reduction Potential: A Theoretical Study on Cyclic Electron-Acceptor Compounds. <i>ChemPhysChem</i> , 2016 , 17, 3881-3890	3.2	11
21	Theoretical description of the Raman spectrum of a vinylene-bridged quaterthiophene oligomer. <i>Journal of Molecular Structure</i> , 2003 , 651-653, 657-664	3.4	9
20	Experimental and theoretical studies into the structural perturbations between neutral, oxidised and reduced forms of 1,4-dithiinoquinoxalinederivatives. <i>Journal of Materials Chemistry</i> , 2000 , 10, 2448-2457		9
19	The First sulfur-containing twin-DCNQI-type acceptor. <i>Advanced Materials</i> , 1994 , 6, 765-768	24	9
18	Theoretical eht study of propene adsorption on model clusters of first series transition metal oxides and MgO. <i>Journal of Molecular Catalysis</i> , 1985 , 30, 81-93		8
17	A proposal for a branching mechanism in medium-sized cycloalkanes: MINDO/3 study of the hypersurface for isomerization of cyclohexylium to 1-methylcyclopentylum ion. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1986 , 49-53		8

16	Effects of Carbon-sp ³ Bridging on the Electronic Properties of Oligothiophenes. <i>Synthetic Metals</i> , 1999 , 101, 602-603	3.6	7
15	Molecular and electronic structure of a largely extended tetracyanoquinodimethane. <i>Synthetic Metals</i> , 1995 , 70, 1031-1032	3.6	7
14	A theoretical study of the molecular and electronic structure of benzoannulated tetracyanoquinodimethanes. <i>Journal of Materials Chemistry</i> , 1995 , 5, 1697-1705		7
13	Theoretical EHT study of propene adsorption on model clusters. <i>Journal of Molecular Catalysis</i> , 1986 , 34, 47-55		7
12	6,11-Bis(dicyanomethylene)-12-methylbenzo[b]phenoxazine and 6,11-dicyanimino-12-methylbenzo[b]phenoxazine as novel donor-acceptor systems. <i>Journal of Materials Chemistry</i> , 1995 , 5, 1563-1570		6
11	Theoretical EHT study of oxidative coupling of methane on pure MgO and MgO doped with Li and Na. <i>Journal of Molecular Catalysis</i> , 1991 , 64, 191-200		6
10	Theoretical and structural studies of lithium cyclic amide conformations. Monomers and aggregates. <i>Perkin Transactions II RSC</i> , 2000 , 1619-1624		5
9	Theoretical eht study of isobutene adsorption on model clusters of first series transition metal oxides and MgO. <i>Journal of Molecular Catalysis</i> , 1988 , 43, 303-314		4
8	Theoretical insights into the structural, electronic and optical properties of benzotrithiophene-based hole-transporting materials. <i>Theoretical Chemistry Accounts</i> , 2017 , 136, 1	1.9	3
7	A study by spectroelectrochemical FTIR and density functional theory calculations of the reversible complexing ability of an electroactive tetrathiafulvalene crown. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 1188-95	2.8	3
6	Valence electronic structure of C ₆₀ : Theoretical analysis of photoemission data. <i>Synthetic Metals</i> , 1993 , 56, 3246-3251	3.6	2
5	Acene-type donors bearing one 1,3-dithiole ring. <i>Synthetic Metals</i> , 1999 , 102, 1635-1636	3.6	1
4	Influence of nitrogen substitution on the electronic band structure of poly(peri-naphthalene). <i>Synthetic Metals</i> , 1995 , 69, 705-706	3.6	1
3	Benzoannulated quinone-type electron acceptors: evolution of the molecular and electronic structures upon reduction. <i>Computational and Theoretical Chemistry</i> , 1998 , 426, 135-143		
2	Geometric and electronic structure of dithiapyranylidine: evolution upon oxidation. <i>Synthetic Metals</i> , 1993 , 57, 4572-4578	3.6	
1	MINDO/3 Study of the Rearrangement of 1-Methylcyclohexyl Cation to 1,2-Dimethylcyclopentyl Cation. <i>Journal of Computational Chemistry</i> , 1986 , 7, 417-427	3.5	