Pedro M Viruela

List of Publications by Year in Descending Order

100 papers	3,617 citations	36 h-index	57 g-index
101 ext. papers	3,755 ext. citations	5.9 avg, IF	4.61 L-index

#	Paper	IF	Citations
100	Helical supramolecular polymerization of C3-symmetric amides and retroamides: on the origin of cooperativity and handedness. *Chemical Communications*, **2016**, 52, 6907-10	5.8	21
99	Non-centrosymmetric homochiral supramolecular polymers of tetrahedral subphthalocyanine molecules. *Angewandte Chemie - International Edition*, **2015**, 54, 2543-7	16.4	51
98	Theoretical insight on novel donor-acceptor exTTF-based dyes for dye-sensitized solar cells. *Journal of Molecular Modeling*, **2014**, 20, 2188	2	2
97	Tuning the electronic properties of nonplanar exTTF-based push-pull chromophores by aryl substitution. *Journal of Organic Chemistry*, **2012**, 77, 10707-17	4.2	40
96	Carbonyl-functionalized quaterthiophenes: a study of the vibrational Raman and electronic absorption/emission properties guided by theoretical calculations. *ChemPhysChem*, **2012**, 13, 168-76	3.2	8
95	Functionalized pentacenes: a combined theoretical, Raman and UV□Vis spectroscopic study. *Theoretical Chemistry Accounts*, **2011**, 128, 521-530	1.9	19
94	Cooperative supramolecular polymerization and amplification of chirality in C3-symmetrical OPE-based trisamides. *Chemistry - A European Journal*, **2011**, 17, 7755-9	4.8	67
93	Oligothienoacenes versus oligothiophenes: impact of ring fusion on the optical properties. *Physical Chemistry Chemical Physics*, **2011**, 13, 1457-65	3.6	30
92	ExTTF-based dyes absorbing over the whole visible spectrum. *Organic Letters*, **2011**, 13, 604-7	6.2	28
91	Diferrocenyl oligothiophene wires: Raman and quantum chemical study of valence-trapped cations. *Journal of Chemical Physics*, **2011**, 135, 234705	3.9	2
90	Quinoidal oligothiophenes: towards biradical ground-state species. *Chemistry - A European Journal*, **2010**, 16, 470-84	4.8	63
89	Neutral and oxidized triisopropylsilyl end-capped oligothienoacenes: a combined electrochemical, spectroscopic, and theoretical study. *Chemistry - A European Journal*, **2010**, 16, 5481-91	4.8	24
88	FT Raman and DFT study on a series of all-anti oligothienoacenes end-capped with triisopropylsilyl groups. *ChemPhysChem*, **2009**, 10, 3069-76	3.2	11
87	Lowest triplet excited states of a novel heteroleptic iridium(III) complex and their role in the emission colour. *Computational and Theoretical Chemistry*, **2009**, 912, 21-26		17
86	From linear quaterthiophene to sulflower: A comparative theoretical study. *Computational and Theoretical Chemistry*, **2009**, 912, 27-31		9
85	Controlled self-assembly of electron donor nanotubes. *Organic Letters*, **2009**, 11, 4524-7	6.2	24
84	Weighting non-covalent forces in the molecular recognition of C(60). Relevance of concave-convex complementarity. *Chemical Communications*, **2008**, 4567-9	5.8	68

83	Theoretical study of oligomeric alumatranes present in the chemistry of materials from micro to mesoporous molecular sieves and alumina composites. *Computational and Theoretical Chemistry*, **2008**, 850, 94-104		5
82	Concave tetrathiafulvalene-type donors as supramolecular partners for fullerenes. *Angewandte Chemie - International Edition*, **2007**, 46, 1847-51	16.4	113
81	On the biradicaloid nature of long quinoidal oligothiophenes: experimental evidence guided by theoretical studies. *Angewandte Chemie - International Edition*, **2007**, 46, 9057-61	16.4	139
80	Molecular precursors of mesostructured silica materials in the atrane route: A DFT/GIAO/NBO theoretical study. *Computational and Theoretical Chemistry*, **2007**, 822, 89-102		12
79	Predicting the activity of single isolated Lewis acid sites in solid catalysts. *Chemistry - A European Journal*, **2006**, 12, 7067-77	4.8	86
78	Magnetic Properties of Quinoidal Oligothiophenes: More Than Good Candidates for Ambipolar Organic Semiconductors?. *Advanced Functional Materials*, **2006**, 16, 531-536	15.6	41
77	Stable single-layer light-emitting electrochemical cell using 4,7-diphenyl-1,10-phenanthroline-bis(2-phenylpyridine)iridium(III) hexafluorophosphate. *Journal of the American Chemical Society*, **2006**, 128, 14786-7	16.4	177
76	Magnetic and Conductive Properties of Quinoidal Oligothiophenes. *Chemistry of Materials*, **2006**, 18, 1539-1545	9.6	32
75	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
74	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
73	Mesitylthio-oligothiophenes in various redox states. Molecular and electronic views as offered by spectroscopy and theory. *Journal of Physical Chemistry A*, **2005**, 109, 11275-84	2.8	19
72	A multisite molecular mechanism for Baeyer-Villiger oxidations on solid catalysts using environmentally friendly H2O2 as oxidant. *Chemistry - A European Journal*, **2005**, 11, 6905-15	4.8	80
71	Spectroscopic and theoretical study of the molecular and electronic structures of a terthiophene-based quinodimethane. *ChemPhysChem*, **2004**, 5, 529-39	3.2	43
70	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
69	Reaction intermediates in acid catalysis by zeolites: prediction of the relative tendency to form alkoxides or carbocations as a function of hydrocarbon nature and active site structure. *Journal of the American Chemical Society*, **2004**, 126, 3300-9	16.4	163
68	Theoretical description of the Raman spectrum of a vinylene-bridged quaterthiophene oligomer. *Journal of Molecular Structure*, **2003**, 651-653, 657-664	3.4	9
67	UVVis, IR, Raman and theoretical characterization of a novel quinoid oligothiophene molecular material. *Journal of Molecular Structure*, **2003**, 651-653, 665-673	3.4	10
66	Nitro-functionalized oligothiophenes as a novel type of electroactive molecular material: spectroscopic, electrochemical, and computational study. *Journal of the American Chemical Society*, **2003**, 125, 2524-34	16.4	101

65	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
64	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
63	Electronic Transitions in Tetrathiafulvalene and Its Radical Cation: A Theoretical Contribution. *Journal of Physical Chemistry A*, **2002**, 106, 631-640	2.8	40
62	Combined Spectroelectrochemical and Theoretical Study of a Vinylene-Bridged Sexithiophene Cooligomer: Analysis of the Electron Delocalization and of the Electronic Defects Generated upon Doping. *Journal of Physical Chemistry B*, **2002**, 106, 3872-3881	3.4	60
61	Cluster and periodic calculations of the ethene protonation reaction catalyzed by theta-1 zeolite: influence of method, model size, and structural constraints. *Chemistry - A European Journal*, **2001**, 7, 1295-303	4.8	26
60	The skeletal isomerization of but-1-ene catalyzed by theta-1 zeolite. *Physical Chemistry Chemical Physics*, **2001**, 3, 3235-3239	3.6	26
59	Influence of the Local Geometry of Zeolite Active Sites and Olefin Size on the Stability of Alkoxide Intermediates. *Journal of Physical Chemistry B*, **2001**, 105, 11169-11177	3.4	59
58	Theoretical and structural studies of lithium cyclic amide conformations. Monomers and aggregates. *Perkin Transactions II RSC*, **2000**, 1619-1624		5
57	Electrochemical molecular recognition of silvercation by electropolymerised thieno[3?,4?:5,6][1,4]dithiino[2,3-b]quinoxaline:a joint experimental and theoretical study. *Journal of Materials Chemistry*, **2000**, 10, 2458-2465		7
56	Ab initio and density-functional theory study of zeolite-catalyzed hydrocarbon reactions: hydride transfer, alkylation and disproportionation. *Physical Chemistry Chemical Physics*, **2000**, 2, 3327-3333	3.6	30
55	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
54	Theoretical Study of Bimolecular Reactions between Carbenium Ions and Paraffins: The Proposal of a Common Intermediate for Hydride Transfer, Disproportionation, Dehydrogenation, and Alkylation. *Journal of Physical Chemistry B*, **1999**, 103, 7809-7821	3.4	38
53	Cluster and periodic abinitio study of the ethane-ethene hydride transfer reaction catalyzed by acid chabazite. Is the cluster model able to describe accurately the host guest interactions?. *Physical Chemistry Chemical Physics*, **1999**, 1, 537-543	3.6	30
52	Flexibility of TTF. a theoretical study. *Synthetic Metals*, **1999**, 103, 1991-1992	3.6	34
51	Effects of Carbon-sp3 Bridging on the Electronic Properties of Oligothiophenes. *Synthetic Metals*, **1999**, 101, 602-603	3.6	7
50	Benzoannulated quinone-type electron acceptors: evolution of the molecular and electronic structures upon reduction. *Computational and Theoretical Chemistry*, **1998**, 426, 135-143		
49	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
48	Difficulties of density functional theory in predicting the torsional potential of 2,2?-bithiophene **1998**, 70, 303-312		31

47	Structural incorporation of nitrogen into zeolites, and alpos: ab initio molecular orbital calculations on stability and basicity. *Journal of Molecular Catalysis A*, **1998**, 133, 241-250		16
46	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
45	A Theoretical Study of the Mechanism of the Hydride Transfer Reaction between Alkanes and Alkenes Catalyzed by an Acidic Zeolite. *Journal of Physical Chemistry A*, **1998**, 102, 9863-9868	2.8	41
44	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
43	Application of SQMFF Vibrational Calculations to Transition States: DFT and ab Initio Study of the Kinetics of Methyl Azide and Ethyl Azide Thermolysis. *Journal of Physical Chemistry A*, **1998**, 102, 1146-1151	2.8	12
42	Theoretical Study of the Mechanism of Zeolite-Catalyzed Isomerization Reactions of Linear Butenes. *Journal of Physical Chemistry A*, **1998**, 102, 982-989	2.8	90
41	Reaction of C60with Sultines: Synthesis, Electrochemistry, and Theoretical Calculations of Organofullerene Acceptors. *Journal of Organic Chemistry*, **1997**, 62, 7585-7591	4.2	50
40	Activation of Molecules in Confined Spaces: An Approach to Zeolite–Guest Supramolecular Systems. *Journal of Physical Chemistry B*, **1997**, 101, 4575-4582	3.4	68
39	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
38	Theoretical Study on the Mechanism of the Hydride Transfer Reaction between Alkanes and Alkylcarbenium Ions. *Journal of Physical Chemistry B*, **1997**, 101, 10069-10074	3.4	31
37	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
36	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
35	Quantum chemistry calculations on the effect of electron confinement upon the frontier molecular orbitals of ethylene and benzene in sodalite. Implications on reactivity. *Chemical Physics Letters*, **1997**, 264, 565-572	2.5	9
34	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
33	Influence of Benzoannulation on the Molecular and Electronic Structures of Tetracyanoquinodimethanes. *The Journal of Physical Chemistry*, **1996**, 100, 6138-6146		34
32	Theoretical study of the mechanism of branching rearrangement of carbenium ions. *Applied Catalysis A: General*, **1996**, 146, 207-223	5.1	17
31	Theoretical Study on the Mechanism of the Superacid-Catalyzed Unimolecular Isomerization of n-Butane and 1-Butene. *The Journal of Physical Chemistry*, **1996**, 100, 633-637		39
30	A Theoretical Study on the Mechanism of the Superacid-Catalyzed Unimolecular Isomerization of n-Alkanes and n-Alkenes. Comparison between ab Initio and Density Functional Results. *The Journal of Physical Chemistry*, **1996**, 100, 16514-16521		23

29	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
28	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
27	Molecular and electronic structure of a largely extended tetracyanoquinodimethane. *Synthetic Metals*, **1995**, 70, 1031-1032	3.6	7
26	6,11-Bis(dicyanomethylene)-12-methylbenzo[b]phenoxazine and 6,11-dicyanimino-12-methylbenzo[b]phenoxazine as novel donor□cceptor systems. *Journal of Materials Chemistry*, **1995**, 5, 1563-1570		6
25	Formation of Surface Methoxy Groups on H-Zeolites from Methanol. A Quantum Chemical Study. *The Journal of Physical Chemistry*, **1995**, 99, 13224-13231		75
24	New functionalized tetrathiafulvalenes: X-ray crystal structures and physico-chemical properties of TTF□(O)NMe2 and TTF□(O)□□4H9: a joint experimental and theoretical study. *Journal of Materials Chemistry*, **1995**, 5, 1689-1696		50
23	A theoretical study of the molecular and electronic structure of benzoannulated tetracyanoquinodimethanes. *Journal of Materials Chemistry*, **1995**, 5, 1697-1705		7
22	Ab Initio Determination of the Geometric Structure and Internal Rotation Potential of 2,2SBithiophene. *The Journal of Physical Chemistry*, **1995**, 99, 4955-4963		111
21	Influence of nitrogen substitution on the electronic band structure of poly(peri-naphthalene). *Synthetic Metals*, **1995**, 69, 705-706	3.6	1
20	A quantum-chemical study of para/ortho-toluene alkylation by adsorbed methoxy species on zeolites. *Journal of Molecular Catalysis A*, **1995**, 100, 75-85		16
19	Electronic Confinement of Molecules in Microscopic Pores. A New Concept Which Contributes to the Explanation of the Catalytic Activity of Zeolites. *The Journal of Physical Chemistry*, **1994**, 98, 10863-10870		128
18	Orbital-controlled reactions catalysed by zeolites: Electrophilic alkylation of aromatics. *Journal of Physical Organic Chemistry*, **1994**, 7, 364-370	2.1	12
17	The First sulfur-containing twin-DCNQI-type acceptor. *Advanced Materials*, **1994**, 6, 765-768	24	9
16	Single-Component Donor-Acceptor Organic Semiconductors Derived from TCNQ. *Journal of Organic Chemistry*, **1994**, 59, 4618-4629	4.2	42
15	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
14	Acid softness and hardness in large-pore zeolites as a determinant parameter to control selectivity in orbital-controlled reactions. *Journal of the American Chemical Society*, **1994**, 116, 134-142	16.4	48
13	Theoretical calculations on the valence electronic structure of naphthalocyanine: comparison with experimental photoemission data. *Synthetic Metals*, **1993**, 57, 4513-4518	3.6	2
12	Valence electronic structure of C60: Theoretical analysis of photoemission data. *Synthetic Metals*, **1993**, 56, 3246-3251	3.6	2

11	Geometric and electronic structure of dithiapyranylidine: evolution upon oxidation. *Synthetic Metals*, **1993**, 57, 4572-4578	3.6	
10	Ab initio molecular orbital calculations of the protonation of propylene and isobutene by acidic hydroxyl groups of isomorphously substituted zeolites. *The Journal of Physical Chemistry*, **1993**, 97, 13713-13719		91
9	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
8	ISomerization of xylene: MINDO/3 study of the cyclization of benzenium cation into bicyclo[3.1.0]hexenyl cation. *Journal of Molecular Catalysis*, **1989**, 52, 277-295		1
7	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
6	A theoretical study of the interaction of acetylene with copper and silver monoions. *The Journal of Physical Chemistry*, **1988**, 92, 4853-4859		30
5	Molecular conformation and electronic structure of 1,1Sbipyrrole. an ab initio approach. *Chemical Physics Letters*, **1986**, 130, 285-290	2.5	6
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