# Pedro M Viruela

List of Publications by Year
in descending order



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|---|---|---|---|
| 101 papers | 4,022 citations | 94433 37 h-index | 123424 61 g-index |
| 101 all docs | 101 docs citations | 101 times ranked | 3936 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | 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, 14786-14787. | 13.7 | 191 |
| 2 | Reaction Intermediates in Acid Catalysis by Zeolites:â€‰ 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, 3300-3309. | 13.7 | 180 |
| 3 | On the Biradicaloid Nature of Long Quinoidal Oligothiophenes: Experimental Evidence Guided by Theoretical Studies. Angewandte Chemie - International Edition, 2007, 46, 9057-9061. | 13.8 | 143 |
| 4 | 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. | 2.9 | 138 |
| 5 | Synthesis, Properties, and Theoretical Characterization of Largely Ï€-Extended Tetrathiafulvalene Derivatives with Quinonoid Structures. Journal of Organic Chemistry, 1998, 63, 1268-1279. | 3.2 | 128 |
| 6 | Ab Initio Determination of the Geometric Structure and Internal Rotation Potential of 2,2'-Bithiophene. The Journal of Physical Chemistry, 1995, 99, 4955-4963. | 2.9 | 117 |
| 7 | Concave Tetrathiafulvalene-Type Donors as Supramolecular Partners for Fullerenes. Angewandte Chemie - International Edition, 2007, 46, 1847-1851. | 13.8 | 117 |
| 8 | Predicting the Activity of Single Isolated Lewis Acid Sites in Solid Catalysts. Chemistry - A European Journal, 2006, 12, 7067-7077. | 3.3 | 108 |
| 9 | Nitro-Functionalized Oligothiophenes as a Novel Type of Electroactive Molecular Material:Â Spectroscopic, Electrochemical, and Computational Study. Journal of the American Chemical Society, 2003, 125, 2524-2534. | 13.7 | 106 |
| 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. | 2.9 | 105 |
| 11 | Theoretical Study of the Mechanism of Zeolite-Catalyzed Isomerization Reactions of Linear Butenes. Journal of Physical Chemistry A, 1998, 102, 982-989. | 2.5 | 105 |
| 12 | Geometric Structure and Torsional Potential of Biisothianaphthene. A Comparative DFT and ab Initio Study. Journal of the American Chemical Society, 1997, 119, 1360-1369. | 13.7 | 99 |
| 13 | Synthesis and Electrochemistry of Electronegative Spiroannelated Methanofullerenes:Â 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. | 13.7 | 95 |
| 14 | A Multisite Molecular Mechanism for Baeyer-Villiger Oxidations on Solid Catalysts Using Environmentally Friendly H2O2 as Oxidant. Chemistry - A European Journal, 2005, 11, 6905-6915. | 3.3 | 94 |
| 15 | Formation of Surface Methoxy Groups on H-Zeolites from Methanol. A Quantum Chemical Study. The Journal of Physical Chemistry, 1995, 99, 13224-13231. | 2.9 | 88 |
| 16 | Cooperative Supramolecular Polymerization and Amplification of Chirality in C<sub>3</sub>â€Symmetrical OPEâ€Based Trisamides. Chemistry - A European Journal, 2011, 17, 7755-7759. | 3.3 | 78 |
| 17 | Quinoidal Oligothiophenes: Towards Biradical Groundâ€State Species. Chemistry - A European Journal, 2010, 16, 470-484. | 3.3 | 74 |
| 18 | Activation of Molecules in Confined Spaces:Â An Approach to Zeoliteâˆ'Guest Supramolecular Systems. Journal of Physical Chemistry B, 1997, 101, 4575-4582. | 2.6 | 72 |

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| 19 | Weighting non-covalent forces in the molecular recognition of C60. Relevance of concaveâ€“convex complementarity. Chemical Communications, 2008, , 4567. | 4.1 | 71 |
| 20 | 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. | 2.6 | 66 |
| 21 | Combined Spectroelectrochemical and Theoretical Study of a Vinylene-Bridged Sexithiophene Cooligomer:Â Analysis of the Ï€-Electron Delocalization and of the Electronic Defects Generated upon Doping. Journal of Physical Chemistry B, 2002, 106, 3872-3881. | 2.6 | 63 |
| 22 | Nonâ€Centrosymmetric Homochiral Supramolecular Polymers of Tetrahedral Subphthalocyanine Molecules. Angewandte Chemie - International Edition, 2015, 54, 2543-2547. | 13.8 | 63 |
| 23 | Reaction of C60with Sultines:Â Synthesis, Electrochemistry, and Theoretical Calculations of Organofullerene Acceptors. Journal of Organic Chemistry, 1997, 62, 7585-7591. | 3.2 | 59 |
| 24 | Donor-Ï€-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. | 3.3 | 56 |
| 25 | 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. | 13.7 | 55 |
| 26 | New 1,3-dithiol-2-ylidene donorâ€“Ï€â€“acceptor chromophores with intramolecular charge-transfer properties, and related donorâ€“Ï€â€“donor molecules: synthesis, electrochemistry, X-ray crystal structures, non-linear optical properties and theoretical calculations. Journal of Materials Chemistry, 1998, 8, 1173-1184. | 6.7 | 53 |
| 27 | New functionalized tetrathiafulvalenes: X-ray crystal structures and physico-chemical properties of TTFâ€“C(O)NMe2and TTFâ€“C(O)â€“Oâ€“C4H9: a joint experimental and theoretical study. Journal of Materials Chemistry, 1995, 5, 1689-1696. | 6.7 | 52 |
| 28 | 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. | 2.5 | 48 |
| 29 | Single-Component Donor-Acceptor Organic Semiconductors Derived from TCNQ. Journal of Organic Chemistry, 1994, 59, 4618-4629. | 3.2 | 47 |
| 30 | 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. | 2.6 | 47 |
| 31 | Spectroscopic and Theoretical Study of the Molecular and Electronic Structures of a Terthiophene-Based Quinodimethane. ChemPhysChem, 2004, 5, 529-539. | 2.1 | 46 |
| 32 | Theoretical Study of Bimolecular Reactions between Carbenium Ions and Paraffins:Â The Proposal of a Common Intermediate for Hydride Transfer, Disproportionation, Dehydrogenation, and Alkylation. Journal of Physical Chemistry B, 1999, 103, 7809-7821. | 2.6 | 45 |
| 33 | Tuning the Electronic Properties of Nonplanar exTTF-Based Pushâ€“Pull Chromophores by Aryl Substitution. Journal of Organic Chemistry, 2012, 77, 10707-10717. | 3.2 | 44 |
| 34 | Theoretical Study on the Mechanism of the Superacid-Catalyzed Unimolecular Isomerization ofn-Butane and 1-Butene. The Journal of Physical Chemistry, 1996, 100, 633-637. | 2.9 | 43 |
| 35 | Electronic Transitions in Tetrathiafulvalene and Its Radical Cation:â€‰ A Theoretical Contribution. Journal of Physical Chemistry A, 2002, 106, 631-640. | 2.5 | 42 |
| 36 | Magnetic Properties of Quinoidal Oligothiophenes: More Than Good Candidates for Ambipolar Organic Semiconductors?. Advanced Functional Materials, 2006, 16, 531-536. | 14.9 | 42 |

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| 37 | Theoretical Study on the Mechanism of the Hydride Transfer Reaction between Alkanes and Alkylcarbenium Ions. Journal of Physical Chemistry B, 1997, 101, 10069-10074. | 2.6 | 37 |
| 38 | Flexibility of TTF. a theoretical study. Synthetic Metals, 1999, 103, 1991-1992. | 3.9 | 37 |
| 39 | Influence of Benzoannulation on the Molecular and Electronic Structures of Tetracyanoquinodimethanes. The Journal of Physical Chemistry, 1996, 100, 6138-6146. | 2.9 | 36 |
| 40 | 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. | 2.8 | 36 |
| 41 | Cluster and periodic ab initio study of the ethane-ethene hydride transfer reaction catalyzed by acid chabazite. Is the cluster model able to describe accurately the hostâ€“guest interactions?. Physical Chemistry Chemical Physics, 1999, 1, 537-543. | 2.8 | 35 |
| 42 | Difficulties of density functional theory in predicting the torsional potential of 2,2?-bithiophene. , 1998, 70, 303-312. | | 34 |
| 43 | A theoretical study of the interaction of acetylene with copper and silver monoions. The Journal of Physical Chemistry, 1988, 92, 4853-4859. | 2.9 | 33 |
| 44 | Magnetic and Conductive Properties of Quinoidal Oligothiophenes. Chemistry of Materials, 2006, 18, 1539-1545. | 6.7 | 32 |
| 45 | The skeletal isomerization of but-1-ene catalyzed by theta-1 zeolite. Physical Chemistry Chemical Physics, 2001, 3, 3235-3239. | 2.8 | 30 |
| 46 | Oligothienoacenes versus oligothiophenes: impact of ring fusion on the optical properties. Physical Chemistry Chemical Physics, 2011, 13, 1457-1465. | 2.8 | 30 |
| 47 | ExTTF-Based Dyes Absorbing over the Whole Visible Spectrum. Organic Letters, 2011, 13, 604-607. | 4.6 | 30 |
| 48 | Helical supramolecular polymerization of C<sub>3</sub>-symmetric amides and retroamides: on the origin of cooperativity and handedness. Chemical Communications, 2016, 52, 6907-6910. | 4.1 | 29 |
| 49 | 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, 1295-1303. | 3.3 | 28 |
| 50 | Highly Conjugatedp-QuinonoidÏ€-Extended Tetrathiafulvalene Derivatives: A Class of Highly Distorted Electron Donors. Chemistry - A European Journal, 2004, 10, 2067-2077. | 3.3 | 28 |
| 51 | Raman and Theoretical Study of the Solvent Effects on the Sizable Intramolecular Charge Transfer in the Pushâ^'Pull 5-(Dimethylamino)-5â€˜-nitro-2,2â€˜-bithiophene. Journal of Physical Chemistry A, 2005, 109, 8724-8731. | 2.5 | 28 |
| 52 | 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. | 3.2 | 27 |
| 53 | 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. | 2.8 | 26 |
| 54 | Controlled Self-Assembly of Electron Donor Nanotubes. Organic Letters, 2009, 11, 4524-4527. | 4.6 | 26 |

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| 55 | A Theoretical Study on the Mechanism of the Superacid-Catalyzed Unimolecular Isomerization ofn-Alkanes andn-Alkenes. Comparison between ab Initio and Density Functional Results. The Journal of Physical Chemistry, 1996, 100, 16514-16521. | 2.9 | 25 |
| 56 | Neutral and Oxidized Triisopropylsilyl Endâ€Capped Oligothienoacenes: A Combined Electrochemical, Spectroscopic, and Theoretical Study. Chemistry - A European Journal, 2010, 16, 5481-5491. | 3.3 | 25 |
| 57 | Functionalized pentacenes: a combined theoretical, Raman and UVâ€“Vis spectroscopic study. Theoretical Chemistry Accounts, 2011, 128, 521-530. | 1.4 | 22 |
| 58 | Synthesis, Characterization, and Theoretical Study of Sulfur-Containing Donorâ^'Acceptor DCNQI Derivatives with Photoinduced Intramolecular Electron Transfer. Journal of Organic Chemistry, 1996, 61, 3041-3054. | 3.2 | 21 |
| 59 | Mesitylthio-Oligothiophenes in Various Redox States. Molecular and Electronic Views as Offered by Spectroscopy and Theory. Journal of Physical Chemistry A, 2005, 109, 11275-11284. | 2.5 | 21 |
| 60 | 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. | 3.2 | 20 |
| 61 | Theoretical study of the mechanism of branching rearrangement of carbenium ions. Applied Catalysis A: General, 1996, 146, 207-223. | 4.3 | 19 |
| 62 | 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. | 13.7 | 18 |
| 63 | A quantum-chemical study of para/ortho-toluene alkylation by adsorbed methoxy species on zeolites. Journal of Molecular Catalysis A, 1995, 100, 75-85. | 4.8 | 18 |
| 64 | A New Type of Ï€-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. | 2.4 | 18 |
| 65 | 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. | 4.8 | 17 |
| 66 | 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. | 1.5 | 17 |
| 67 | Synthesis, properties and charge transfer complexes of covalently attached [60]fullerene-tetrathiafulvalenes. Journal of Physics and Chemistry of Solids, 1997, 58, 1713-1718. | 4.0 | 14 |
| 68 | Orbital-controlled reactions catalysed by zeolites: Electrophilic alkylation of aromatics. Journal of Physical Organic Chemistry, 1994, 7, 364-370. | 1.9 | 13 |
| 69 | The First sulfur-containing twin-DCNQI-type acceptor. Advanced Materials, 1994, 6, 765-768. | 21.0 | 13 |
| 70 | Molecular precursors of mesostructured silica materials in the atrane route: A DFT/GIAO/NBO theoretical study. Computational and Theoretical Chemistry, 2007, 822, 89-102. | 1.5 | 13 |
| 71 | Application of SQMFF Vibrational Calculations to Transition States:Â DFT and ab Initio Study of the Kinetics of Methyl Azide and Ethyl Azide Thermolysis. Journal of Physical Chemistry A, 1998, 102, 1146-1151. | 2.5 | 12 |
| 72 | 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. | 1.2 | 11 |

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| 73 | 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. | 2.6 | 11 |
| 74 | FT Raman and DFT Study on a Series of Allâ€anti Oligothienoacenes Endâ€Capped with Triisopropylsilyl Groups. ChemPhysChem, 2009, 10, 3069-3076. | 2.1 | 11 |
| 75 | From linear quaterthiophene to sulflower: A comparative theoretical study. Computational and Theoretical Chemistry, 2009, 912, 27-31. | 1.5 | 11 |
| 76 | UVâ€“Vis, IR, Raman and theoretical characterization of a novel quinoid oligothiophene molecular material. Journal of Molecular Structure, 2003, 651-653, 665-673. | 3.6 | 10 |
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| 78 | Molecular conformation and electronic structure of 1,1'-bipyrrole. an ab initio approach. Chemical Physics Letters, 1986, 130, 285-290. | 2.6 | 9 |
| 79 | Theoretical description of the Raman spectrum of a vinylene-bridged quaterthiophene oligomer. Journal of Molecular Structure, 2003, 651-653, 657-664. | 3.6 | 9 |
| 80 | 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. | 1.2 | 8 |
| 81 | Theoretical EHT study of propene adsorption on model clusters. Journal of Molecular Catalysis, 1986, 34, 47-55. | 1.2 | 8 |
| 82 | Molecular and electronic structure of a largely extended tetracyanoquinodimethane. Synthetic Metals, 1995, 70, 1031-1032. | 3.9 | 8 |
| 83 | A theoretical study of the molecular and electronic structure of benzoannulated tetracyanoquinodimethanes. Journal of Materials Chemistry, 1995, 5, 1697-1705. | 6.7 | 8 |
| 84 | Effects of Carbon-sp3 Bridging on the Electronic Properties of Oligothiophenes. Synthetic Metals, 1999, 101, 602-603. | 3.9 | 8 |
| 85 | Electrochemical molecular recognition of silver cation by electropolymerised thieno[3â€²,4â€²:5,6][1,4]dithiino[2,3-b]quinoxaline: a joint experimental and theoretical study. Journal of Materials Chemistry, 2000, 10, 2458-2465. | 6.7 | 8 |
| 86 | Carbonylâ€Functionalized Quaterthiophenes: A Study of the Vibrational Raman and Electronic Absorption/Emission Properties Guided by Theoretical Calculations. ChemPhysChem, 2012, 13, 168-176. | 2.1 | 8 |
| 87 | 6,11-Bis(dicyanomethylene)-12-methylbenzo[b]phenoxazine and 6,11-dicyanimino-12-methylbenzo[b]phenoxazine as novel donorâ€“acceptor systems. Journal of Materials Chemistry, 1995, 5, 1563-1570. | 6.7 | 6 |
| 88 | 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. | 1.5 | 6 |
| 89 | Theoretical and structural studies of lithium cyclic amide conformations. Monomers and aggregates. Perkin Transactions II RSC, 2000, , 1619-1624. | 1.1 | 5 |
| 90 | 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. | 1.2 | 4 |

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| 91 | 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, 1188-1195. | 2.5 | 3 |
| 92 | Theoretical insight on novel donor-acceptor exTTF-based dyes for dye-sensitized solar cells. Journal of Molecular Modeling, 2014, 20, 2188. | 1.8 | 3 |
| 93 | MINDO/3 study of the isomerization of 1-methylcyclohexylium ion to 1-ethylcyclopentylium ion. An alternative mechanism for this branching rearrangement. Journal of the Chemical Society Perkin Transactions II, 1987, , 307-311. | 0.9 | 2 |
| 94 | Theoretical calculations on the valence electronic structure of naphthalocyanine: comparison with experimental photoemission data. Synthetic Metals, 1993, 57, 4513-4518. | 3.9 | 2 |
| 95 | Valence electronic structure of C60: Theoretical analysis of photoemission data. Synthetic Metals, 1993, 56, 3246-3251. | 3.9 | 2 |
| 96 | Diferrocenyl oligothiophene wires: Raman and quantum chemical study of valence-trapped cations. Journal of Chemical Physics, 2011, 135, 234705. | 3.0 | 2 |
| 97 | 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. | 1.2 | 1 |
| 98 | Influence of nitrogen substitution on the electronic band structure of poly(peri-naphthalene). Synthetic Metals, 1995, 69, 705-706. | 3.9 | 1 |
| 99 | MINDO/3 Study of the Rearrangement of 1-Methylcyclohexyl Cation to 1,2-Dimethylcyclopentyl Cation. Journal of Computational Chemistry, 1986, 7, 417-427. | 3.3 | 0 |
| 100 | Geometric and electronic structure of dithiapyranylidine: evolution upon oxidation. Synthetic Metals, 1993, 57, 4572-4578. | 3.9 | 0 |
| 101 | Benzoannulated quinone-type electron acceptors: evolution of the molecular and electronic structures upon reduction. Computational and Theoretical Chemistry, 1998, 426, 135-143. | 1.5 | 0 |