Emilio San Fabian

List of Publications by Year
in descending order

99 papers	1,855 citations	279798 23 h-index	302126 39 g-index
103 all docs	103 docs citations	103 times ranked	1765 citing authors

#	Article	IF	Citations
1	Organic Emitters Showing Excited-States Energy Inversion: An Assessment of MC-PDFT and Correlation Energy Functionals Beyond TD-DFT. Computation, 2022, 10, 13.	2.0	5
2	On the mechanism of electrochemical functionalization of carbon nanotubes with different structures with aminophenylphosphonic acid isomers: an experimental and computational approach. Journal of Materials Chemistry A, 2022, 10, 7271-7290.	10.3	4
3	Singletâ€Triplet Excitedâ€State Inversion in Heptazine and Related Molecules: Assessment of TDâ€DFT and ab initio Methods. ChemPhysChem, 2021, 22, 553-560.	2.1	45
4	Energy calculations for potassium vs sodium selectivity on potassium channel: an ab initio study. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	0
5	Probability distribution for heat exchange in plastic deformation. Physical Review E, 2021, 104, 034101.	2.1	0
6	peri-Acenoacene molecules: tuning of the singlet and triplet excitation energies by modifying their radical character. Physical Chemistry Chemical Physics, 2021, 23, 24016-24028.	2.8	5
7	Nonempirical (doubleâ€hybrid) density functionals applied to atomic excitation energies: A systematic basis set investigation. International Journal of Quantum Chemistry, 2020, 120, e26193.	2.0	10
8	Investigating the (Poly)Radicaloid Nature of Real-World Organic Compounds with DFT-Based Methods. Journal of Physical Chemistry A, 2020, 124, 3590-3600.	2.5	7
9	Post-synthetic efficient functionalization of polyaniline with phosphorus-containing groups. Effect of phosphorus on electrochemical properties. European Polymer Journal, 2019, 119, 272-280.	5.4	21
10	Electron enrichment of zigzag edges in armchairâ€“oriented graphene nanoâ€“ribbons increases their stability and induces pinning of the Fermi level. Carbon, 2019, 154, 211-218.	10.3	7
11	Transport and Optical Gaps in Amorphous Organic Molecular Materials. Molecules, 2019, 24, 609.	3.8	0
12	Emerging DFT Methods and Their Importance for Challenging Molecular Systems with Orbital Degeneracy. Computation, 2019, 7, 62.	2.0	5
13	Towards understanding the active sites for the ORR in N-doped carbon materials through fine-tuning of nitrogen functionalities: an experimental and computational approach. Journal of Materials Chemistry A, 2019, 7, 24239-24250.	10.3	87
14	The role of topology in organic molecules: origin and comparison of the radical character in linear and cyclic oligoacenes and related oligomers. Physical Chemistry Chemical Physics, 2018, 20, 7112-7124.	2.8	39
15	Conductance through the armchair graphene nanoribbons 9-AGNR: Strong dependence on contact to leads. Physical Review B, 2018, 98, .	3.2	7
16	Are Electron Affinity and Ionization Potential Intrinsic Parameters to Predict the Electron or Hole Acceptor Character of Amorphous Molecular Materials?. Journal of Physical Chemistry Letters, 2017, 8, 2445-2449.	4.6	40
17	The application of TD-DFT to excited states of a family of TPD molecules interesting for optoelectronic use. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	2
18	Theoretical Study of Cyclic Pyrene Oligomers and Their Resemblance with Cyclic Paraphenylenes: Disclosing Structureâ€“Property Relationships for Cyclic Nanorings. Journal of Physical Chemistry C, 2016, 120, 22069-22078.	3.1	4

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19	Herringbone Pattern and CHâ€“Ï€ Bonding in the Crystal Architecture of Linear Polycyclic Aromatic Hydrocarbons. ChemPhysChem, 2016, 17, 3548-3557.	2.1	23
20	Competition for water between protein (from Haloferax mediterranei) and cations $$hbox {Na}^+$$ Na + and $$hbox {K}^+$$ K + : a quantum approach to problem. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	4
21	One step-synthesis of highly dispersed iron species into silica for propylene epoxidation with dioxygen. Journal of Catalysis, 2016, 338, 154-167.	6.2	30
22	Can model Hamiltonians describe the electronâ€“electron interaction inÏ€-conjugated systems?: PAH and graphene. Journal of Physics Condensed Matter, 2015, 27, 463001.	1.8	10
23	Intraâ€•and Intermolecular Dispersion Interactions in [n]Cycloparaphenylenes: Do They Influence Their Structural and Electronic Properties?. ChemPhysChem, 2015, 16, 1520-1528.	2.1	15
24	Role of potassium orbitals in the metallic behavior of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">K</mml:mi><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">picene</mml:mi></mml:math>. Physical Review B, 2014, 90, .	3.2	1
25	Theoretical insights on electron donorâ€“acceptor interactions involving carbon dioxide. Chemical Physics Letters, 2014, 601, 98-102.	2.6	14
26	Cyclobutadiene automerization and rotation of ethylene: Energetics of the barriers by using Spinâ€polarized wave functions. Journal of Computational Chemistry, 2014, 35, 1356-1363.	3.3	3
27	Improvements in DFT Calculations of Spinâ€“Spin Coupling Constants. Journal of Chemical Theory and Computation, 2014, 10, 4938-4949.	5.3	31
28	Polarizedâ€“unpolarized ground state of small polycyclic aromatic hydrocarbons. International Journal of Quantum Chemistry, 2013, 113, 815-819.	2.0	8
29	Exponential decay of spin-spin correlation between distant defect states produced by contour hydrogenation of polycyclic aromatic hydrocarbon molecules. Physical Review B, 2013, 87, .	3.2	6
30	Spin alignment of extra electrons in K-phenanthrene clusters taken from the crystalline tripotassium-intercalated phenanthrene structure. Physical Review B, 2012, 85, .	3.2	8
31	PPP Hamiltonian for polar polycyclic aromatic hydrocarbons. European Physical Journal B, 2011, 81, 253-262.	1.5	7
32	On the actual nature of the anti-ferromagnetism shown by unrestricted calculations on conjugated hydrocarbon rings. European Physical Journal D, 2011, 64, 239-248.	1.3	5
33	Abnormal stress drop at the yield point of aluminum nanowires: A molecular dynamics study. Physical Review B, 2011, 83, .	3.2	16
34	Fit of Pariser-Parr-Pople and Hubbard model Hamiltonians to charge and spin states of polycyclic aromatic hydrocarbons. Physical Review B, 2010, 81, .	3.2	25
35	Non-Gaussian tails in the probability distribution function of heat exchanged during isothermal stretching of aluminum and gold nanowires. Physical Review E, 2009, 80, 030105.	2.1	3
36	Magnetic molecules created by hydrogenation of polycyclic aromatic hydrocarbons. Physical Review B, 2009, 79, .	3.2	14

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37	On the existence of a spin-polarized state in the n-periacene molecules. Chemical Physics Letters, 2009, 480, 26-30.	2.6	35
38	Magnetism in hydroâ€•and dehydrogenated benzene. Physica Status Solidi C: Current Topics in Solid State Physics, 2009, 6, 2139-2144.	0.8	6
39	On the stressâ€strain curves in gold and aluminum nanowires. Physica Status Solidi C: Current Topics in Solid State Physics, 2009, 6, 2119-2122.	0.8	5
40	Asymmetry between Absorption and Photoluminescence Line Shapes of TPD: Spectroscopic Fingerprint of the Twisted Biphenyl Core. Journal of Physical Chemistry A, 2009, 113, 315-324.	2.5	33
41	Effects of methods and basis set on ab initio calculations of electronic transport through hydrogenated Pt nanocontacts. International Journal of Quantum Chemistry, 2008, 108, 1637-1644.	2.0	6
42	Stress-strain curves of aluminum nanowires: Fluctuations in the plastic regime and absence of hardening. Physical Review B, 2008, 78, .	3.2	7
43	Hubbard Hamiltonian for the hydrogen molecule. Physical Review B, 2007, 75, .	3.2	21
44	Theoretical investigation of excited states of molecules. An application on the nitrogen molecule. Theoretical Chemistry Accounts, 2007, 118, 637-642.	1.4	8
45	The Colleâ€“Salvetti Wavefunction Revisited: a Comparison Between Three Approaches for Obtaining the Correlation Energy. Theoretical Chemistry Accounts, 2006, 115, 334-342.	1.4	8
46	Molecular Electronics with Gaussian98/03. Computational Chemistry - Reviews of Current Trends, 2005, , 1-46.	0.4	7
47	Electronic transport and vibrational modes in a small molecular bridge:H2in Pt nanocontacts. Physical Review B, 2004, 69, .	3.2	48
48	Conductance fluctuations in metallic nanocontacts. Physical Review B, 2004, 70, .	3.2	1
49	Correlation factor approach to the correlation energy functional. Theoretical Chemistry Accounts, 2004, 111, 1-17.	1.4	5
50	A study with a complete-active-space self-consistent-field plus density functional theory combination: The low-lying bound states of N 2. Theoretical Chemistry Accounts, 2003, 110, 276-283.	1.4	10
51	Analysis of Scanning Tunneling Spectroscopy Experiments from First Principles: The Test Case of C60 Adsorbed on Au(111). ChemPhysChem, 2003, 4, 388-392.	2.1	31
52	DFT calculations of correlation energies for excited electronic states using MCSCF wave functions. International Journal of Quantum Chemistry, 2003, 91, 451-460.	2.0	12
53	First-Principles Phase-Coherent Transport in Metallic Nanotubes with Realistic Contacts. Physical Review Letters, 2003, 90, 106801.	7.8	159
54	Implementing the Keldysh formalism intoab initiomethods for the calculation of quantum transport: Application to metallic nanocontacts. Physical Review B, 2003, 67, .	3.2	76

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55	First-principles approach to electrical transport in atomic-scale nanostructures. Physical Review B, 2002, 66, .	3.2	186
56	An ab initio approach to electrical transport in molecular devices. Nanotechnology, 2002, 13, 378-381.	2.6	13
57	CORRELATED MULTIDETERMINANTAL POTENTIAL ENERGY CURVES FOR DIATOMIC MOLECULES WITH ONE VALENCE-BOND PAIR. Recent Advances in Computational, 2002, , 293-304.	0.8	0
58	STRATEGIC BEHAVIOR AND INFORMATION TRANSMISSION IN A STYLIZED (SO-CALLED CHINOS) GUESSING GAME. International Journal of Modeling, Simulation, and Scientific Computing, 2001, 04, 177-190.	1.4	3
59	New approach to the design of density functionals. Journal of Chemical Physics, 2001, 114, 2022-2026.	3.0	17
60	Mono and multiconfigurational wave functions with DFT correlation energy: the case of fluorine. Computational and Theoretical Chemistry, 2000, 528, 59-64.	1.5	9
61	MCSCF calculations of NMR spinâ€“spin coupling constant of the HF molecule. Journal of Chemical Physics, 2000, 112, 4143-4152.	3.0	28
62	Density-functional study of van der Waals forces on rare-gas diatomics: Hartreeâ€“Fock exchange. Journal of Chemical Physics, 1999, 110, 1916-1920.	3.0	79
63	On the application of the Kohnâ€“Sham theory to the calculation of potential energy curves. Chemical Physics Letters, 1998, 288, 418-422.	2.6	12
64	Theoretical approach to the photodissociation of CCl32+1. Computational and Theoretical Chemistry, 1998, 426, 289-297.	1.5	0
65	Improvement of Multiconfigurational Wave Functions and Energies by Correlation Energy Functionals. Journal of Physical Chemistry A, 1998, 102, 10900-10902.	2.5	15
66	Differences between ab initio and density functional electron densities. International Journal of Quantum Chemistry, 1997, 61, 245-252.	2.0	8
67	Density functional calculations on Jahn-Teller effect of tetrachloromethane cation. , 1997, 61, 533-540.		5
68	Performance of correlation functionals inab initiochemisorption cluster-model calculations: Alkali metals on Si(111). Physical Review B, 1995, 52, 11998-12005.	3.2	6
69	Ab Initio Study of Electronic Structure and Jahn-Teller Effect of Tetrachloromethane Cation. The Journal of Physical Chemistry, 1995, 99, 12135-12140.	2.9	6
70	Automatic numerical integration techniques for polyatomic molecules. Journal of Chemical Physics, 1994, 100, 6520-6534.	3.0	109
71	Symmetry breaking and its influence on the correlation energy for CF4+ and CF32+ ions. International Journal of Quantum Chemistry, 1994, 52, 947-956.	2.0	8
72	Applicability to atoms of a large set of correlation energy functinals. International Journal of Quantum Chemistry, 1994, 52, 1027-1038.	2.0	5

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73	A simple, efficient and more reliable scheme for automatic numerical integration. Computer Physics Communications, 1993, 77, 46-56.	7.5	28
74	Research in Atomic Structure. Lecture Notes in Quantum Chemistry II, 1993, , .	0.3	5
75	Spectroscopic constants of diatomic molecules computed correcting Hartree-Fock or general-valence-bond potential-energy curves with correlation-energy functionals. Physical Review A, 1992, 45, 4407-4420.	2.5	27
76	Results of the correlation energy functionals versus the wavefunction type. Computational and Theoretical Chemistry, 1992, 254, 1-11.	1.5	11
77	A simple, reliable and efficient scheme for automatic numerical integration. Computer Physics Communications, 1992, 70, 271-284.	7.5	29
78	Jahn-Teller effect and dissociation from the ground state of CF4+. Chemical Physics, 1991, 151, 335-342.	1.9	16
79	Theoretical prediction of secondary structures of proteins using recognition factors. Computational and Theoretical Chemistry, 1991, 226, 87-97.	1.5	7
80	Electroreduction of Î²-chloropropiophenone: a study of stability of cis and trans isomers of 1,5-diphenyl-2,6-dioxa[3,3,0]bicyclooctane and on the logical reaction pathway. Computational and Theoretical Chemistry, 1991, 231, 169-174.	1.5	0
81	Prediction of protein secondary structures using a combined method based on the recognition, lim and garnier-osguthorpe-robson algorithms. Computational and Theoretical Chemistry, 1991, 232, 321-336.	1.5	3
82	A density functional for the correlation energy, deduced in the framework of the correlation factor approach. International Journal of Quantum Chemistry, 1991, 40, 23-32.	2.0	41
83	Density-functional formalism and the two-body problem. Physical Review A, 1991, 44, 1549-1553.	2.5	87
84	On the accuracy of correlation energy calculated by the correlation factor method: first- and second-row atoms. Theoretica Chimica Acta, 1990, 77, 207-212.	0.8	3
85	Prediction of the secondary structure and functional sites of major histocompatibility complex molecules. Journal of Molecular Recognition, 1990, 3, 65-73.	2.1	6
86	Calculation of H-H potential energies and fusion rates inPdxH2clusters (x=2,4). Physical Review B, 1990, 42, 4996-4999.	3.2	2
87	Possibility of finding reliable solid-state tight-binding parameters for the Si-N bond through quantum-chemistry calculations. Physical Review B, 1989, 39, 1844-1855.	3.2	16
88	Atomic energy levels from configuration interaction calculations with relativistic corrections. International Journal of Quantum Chemistry, 1989, 35, 325-330.	2.0	3
89	Density functionals and chemical bond, diatomic molecules. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1989, 86, 853-859.	0.2	6
90	Estimation of minima in1A1states of the ozone molecule. International Journal of Quantum Chemistry, 1988, 34, 375-383.	2.0	9

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91	Computer modelling of protein structures. Computational and Theoretical Chemistry, 1988, 166, 129-134.	1.5	2
92	Theoretical study of the stability of species Aî—¸BH3(Aî—»Liâ€¦Ne). Computational and Theoretical Chemistry, 1988, 166, 293-299.	1.5	3
93	Two-configuration potential energy surface for the Ca + HF â†' CaF + H reaction. Chemical Physics, 1987, 114, 241-249.	1.9	6
94	On the structure and stability of the linear complex between Li and CO₂. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1987, 84, 791-794.	0.2	0
95	Covalent-ionic nature of the potential energy surface of the Li-CO2 complex. Theoretica Chimica Acta, 1986, 70, 297-302.	0.8	10
96	Dynamical analysis of correlated wavefunctions. International Journal of Quantum Chemistry, 1986, 30, 853-865.	2.0	3
97	Electron correlation in the Coulomb hole model. Comparison of methods. Journal of Chemical Physics, 1984, 81, 4008-4013.	3.0	15
98	Relative stability of the2 A 1g and2 E g states of the C2H 6 + ion. Theoretica Chimica Acta, 1979, 53, 377-381.	0.8	8
99	Theoretical study of the ethane ionization spectra within the correlation hole model. Theoretica Chimica Acta, 1979, 54, 53-58.	0.8	7